Effect of the grain size and distribution of nanograins on the deformation of nanodomained heterogeneous nickel

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Abstract

We studied the effect of embedded nanograins on the strength and deformation of nanodomained heterogeneous nickel (Ni) via a novel discrete-crystal plasticity model. Nanodomained structures exhibited higher strength than those of heterogeneous lamella structures and rule of mixtures. Due to the mismatch of strengths between the nanograins and coarse grains, geometrically necessary dislocations (GND) accumulated around nanograins and increased with the strain. In addition, smaller nanograins are more effective to generate GND in both nanodomained and heterogeneous lamella structures. These findings shed light on the role of dislocation mechanisms in the plasticity of heterogeneous nanostructured metals.

Key words: Nanodomain; Crystal plasticity; Nanocrystalline; Finite element model

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1. Introduction

Nanostructured metals with microstructure length scales less than 100 nm, such as metallic nanowires, nanocrystalline (NC) metals and metallic nanolayered films, possess superior properties (ultra-high strength, enhanced fatigue strength and strong corrosion resistance) and unique deformation mechanisms compared to conventional metallic materials [1-5]. For metals, strength and ductility as the two key mechanical properties determine their performance in engineering applications. Traditional methods for preparing nanostructured metals can improve their strength while accompanying with the loss of the ductility. For example, the yield strength of NC coppers can be six times higher than that of the coarse grained copper, but their ductility at room temperature is less than 5% [6]. The low ductility of NC metals results from the lack of dislocation accumulations within the nanograins (NG) during the deformation [7, 8].

Recently, Wu et al. developed a new class of nanostructured metals, nanodomained (ND) metals, which contains randomly dispersed nanograins inside the coarser grains [9]. Although the volume fraction of the nanograins is only a few percent, the yield strength of the ND metals is comparable to the pure NC metals, and the elongation can reach the same level as that for coarse grained metals. The exceptional mechanical properties in ND metals is mainly attributed to the small spacing between the nanograins which effectively increases the pinning resistance to the dislocation motion. That leads to the slow motion of dislocations, providing more opportunities for dislocation intersecting each other, and elevating the storage rate of dislocation within the grain [10]. To design and process ductile high strength ND metals, two critical questions are still unanswered: i) what is the grain size effect of nanograins on the strength of the whole ND structure? ii) how can the randomly embedded nanograins affect with the dislocation accumulation and the plastic strain distribution within the coarse grains (CG)?

Here, we use a novel discrete-crystal plasticity finite element (CPFE) model to study the effects of the grain size of nanogrians on the strength and deformation in ND Ni. In addition, we compare the strength of ND Ni with heterogeneous lamella (HL) Ni to explore the influence of the nanograin distribution on the deformation in heterogeneous nanostructured metals.

2. Methodology

A rate-dependent elasto-viscoplastic constitutive model accounting for elastic and plastic deformation of crystals and the underlying kinematic relations [11] is modified to accommodate the discrete CPFE model used in this work. The plastic shear strain rate in each slip system α is calculated with a power-law equation:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left[\frac{|\tau^{\alpha}|}{\tau^{\alpha}_{CRSS}}\right]^{\frac{1}{m}} sign(\tau^{\alpha}) \tag{1}$$

where $\dot{\gamma}_0$ is a reference shear strain rate, τ^{α} and τ^{α}_{CRSS} are resolved shear stress (RSS) and critical resolved shear stress (CRSS) in slip system α, respectively, and m is the strain rate sensitivity exponent.

In the nanograin part, the CRSS is evaluated by our novel discrete dislocation emission model [12, 13], which assumes the plastic strain within nanograins is induced by the slip of dislocations nucleated from the GBs. The CRSS is controlled by the length of GB dislocations, and equals to the stress required for activating the GB dislocation and subsequently gliding across the grain. It follows the generalized extreme value distribution that will be used in equation (1).

Within the CGs, dislocations glide and interact with each other during plastic deformation, forming forest dislocations which impede further dislocation motions. A homogenized strain hardening scheme is used for the CG part, where CRSS of a slip system is calculated based on the evolution of forest dislocation and geometrically necessary dislocation (GND) densities [14]:

$$\tau^{\alpha}_{CRSS} = \chi\mu b\sqrt{\rho^{\alpha}_{for} + \rho^{\alpha}_{GND}} + \tau^{\alpha}_{sub} \tag{2}$$

where χ is a dislocation interaction factor and ρ^{α}_{for} and ρ^{α}_{GND} are forest dislocation and GND densities in slip system α, respectively. τ^{α}_{sub} is the resistance for the dislocation motion contributed from dislocation substructures. The details about the calculations of each term in above equations can be found in Ref. [12, 14, 15].

The preceding constitutive formulations are written as UMAT subroutines implemented in Abaqus. Figure 1 (a) illustrate the mesh for NC Ni calculations and (b) compares the model predicted stress-strain curves at three different grain sizes with experiment results from Ref.[16, 17]. The predicted stress-strain curves achieve quantitative agreement with experiment data in the yield strength, flow stress and the pronounced grain-size effect.

The geometries of the ND and HL models are shown in Figure 2 (a) and (b). In this study, the volume fraction of nanograins in the whole structure is set to be 5%. In that case, the total numbers of nanograins in both ND and HL structures are exactly the same.

3. Results and discussion

Figure 2 (c) shows the stress-strain curves for the ND and HL structures with different NG sizes and different CG orientations. The CG orientations are [100] and [123], which indicate the multiple-slip and single-slip orientations, respectively [18]. For a FCC crystal such as Ni with [100] orientation, eight of the twelve slip systems have the same maximum Schmid factor (0.408). In contrast, only one of the twelve slip systems has the maximum Schmid factor (0.467) for [123] orientation. In addition, we also compare the CPFE calculated results with the rule of mixtures (ROM) $\sigma_{ROM} = \sum V_i \sigma_i$, where V_i is the volume fraction and σ_i is the strength of each single phase. Since the ROM equation was derived based on isostrain condition that assumes each phase sustains the same strain, it predicts the upper limit of the strength of composites [19].

From Figure 2 (c), we see can that the stress-strain curves for HL structures strictly follow the curves predicted by ROM before macroscopic plastic flow. That is because the NG and CG in the HL structures formed two parallel layers and were deformed under isostrain condition [18]. In contrast, the ND structure contain randomly distributed NGs, its strength is the lowest one among those three cases before macroscopic plastic flow. However, in the plastic flow region with the total strain larger than 4%, the strength for ND structure exceed the other two. And the stress predicted by ROM becomes the lowest one. Furthermore, with the strain increases, the difference of the flow stresses becomes larger between the ND structures, HL structures and ROM. In addition, the structures with [123] orientated coarse grains exhibit higher strengths and strain hardening rates than those for [100] orientated coarse grains.

Since the strength of nanograins is much higher than conventional coarse grains according to the Hall-Petch relationship [1], the strengthening mechanism in ND structures should be similar to precipitation hardening, which refers second phase particles in the matrix harden materials by stopping or slow down the motion of dislocations [19]. With the advantage of the CPFE model, we output the average shear strain rate for each case (Figure 2 (d)). We can see that the average shear strain rates for structures with [123] CG are higher than those for structures with [100] CG. Since the average Schmid factor for [123] CG is about 0.185 smaller than that for [100] CG (0.272), higher average shear strain rates are needed for [123] CG to satisfy external applied strain rate. In addition, the variation of average shear strain rates for 50 nm structures is larger than that for the corresponding 7nm structures, although the average values are close to each other. This larger variation of average shear strain rates in 50 nm structures is induced by the wider CRSS distribution for 50 nm nanograins [12], which can trigger higher fluctuations on local plastic deformation. Furthermore, all average shear strain rate curves exhibit the same trend that they gradually raise with the strain before microscopic plastic flow as the stress increases, then drop with the strain (> 2%) during the plastic flow. Based on equation (1), we can see that the drop of the average shear strain rates should be induced by the decline of the ratio between RSS and CRSS. Since the RSS increases with the applied stress during the deformation, the drop of the average shear strain rates must result from the increase of CRSS for each slip system, which is determined by the dislocation density, especially for the GND.

As there were large mismatch of the strengths between the nanograins and CG, the GND should be present accompanied by internal plastic strain gradients during deformation [20]. The comparison of the distributions of the GND for different structures is shown in Figure 3. It is clear that the GND increases with the strain as the maximum GND at 10% strain in Figure 3 (b) is about four times as that at 5% strain in (a). In addition, 7 nm nanograins can generate more GND in the ND structures than 50 nm nanograins shown in Figure 3 (c), as the mismatch of strengths between the 7 nm nanograins and CG is larger than that for 50 nm nanograins. Furthermore, ND structures are more effective to generate GND than HL structures. The major elements in HL structures in Figure 3 (d) exhibit less GND than ND structures in Figure 3 (b) at the same strain and grain size. This high heterogeneous distribution of the GND can produce significant back stress induced work hardening to enhance/retain ductility [7, 8].

4. Conclusions

We studied the effect of embedded nanograins on the strength and deformation of ND Ni via a novel discrete-crystal plasticity model. Our results indicate that ND structures exhibited higher strength than HL structures and ROM during the plastic flow. Due to the mismatch of strengths between the nanograins and coarse grains, GND were accumulated in both ND and HL structures. The smaller nanograins, the higher accumulated dislocation density.

Acknowledgements

This work was supported by NSF CAREER Award (CMMI-1652662). C.Z. also acknowledges support by the XSEDE Award (DMR170093).

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